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CITATION:

Kusakabe, Koichi. An Extension of the Kohn-Sham Equations for the Correlated Electron Systems(New Developments in Strongly Correlated Electron Systems). 物性研究 2001, 76(5): 697-697

ISSUE DATE:

2001-08-20

URL:

http://hdl.handle.net/2433/97036

An Extension of the Kohn-Sham Equations for the Correlated Electron Systems

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Knowledge on the Mott metal-insulator transition and the Kondo effects has revealed that description of several kinds of electron-correlation effects inevitably requires multi-Slater determinants. In this talk, we reconsider possibility of the so-called first-principles approach for the electronic state calculation based on the density functional theory (DFT) as a standard theory for the interacting electron systems showing these interesting correlation effects.

Tractable calculational methods have been developed by utilizing an additional strategy of DFT, *i.e.* the Kohn-Sham scheme. In this formulation, one considers an imaginative non-interacting model system which is assumed to reproduce the single-particle density $n(\mathbf{r})$ of the true ground state. Then, an effective potential problem is obtained, which is described by the Kohn-Sham equation.

In the present theory, we start from an assumption similar to the Kohn-Sham scheme. Namely, we assume existence of an imaginative interacting system which reproduces $n(\mathbf{r})$. Then, we can derive a many-body problem describing the model system as follows.

$$\left\{-\frac{\hbar^2}{2m}\Delta + v_{\rm eff}(\mathbf{r})\right\}\phi_{i\sigma}(\mathbf{r}) = \varepsilon_i\phi_{i\sigma}(\mathbf{r}) \tag{1}$$

$$\left\{\sum_{i\sigma}\varepsilon_i c^\dagger_{i\sigma}c_{i\sigma} + \sum_{ij\sigma}V^{(1)}_{\rm eff}(ij\sigma)c^\dagger_{i\sigma}c_{j\sigma} + {\sum_{ijkl\sigma\sigma'}}' V^{(2)}_{\rm eff}(ijkl;\sigma\sigma')c^\dagger_{i\sigma}c^\dagger_{j\sigma'}c_{k\sigma'}c_{l\sigma} + \hat{H}_{\rm rxc}\right\}|\Psi\rangle = E|\Psi\rangle \tag{2}$$

Here, the effective potential, $v_{\rm eff}$, in eq. (1) is essentially similar to the Kohn-Sham effective potential, but we note that the ground state of this model is determined by solving eq. (2) including a two-particle interaction, $V^{(2)}_{\rm eff}$, and a Hartree-type mean-field, $V^{(1)}_{\rm eff}$. This set of self-consistent equations are determined by a variational method.

To obtain formula for $v_{\rm eff}$, $V^{(1)}_{\rm eff}$ and $V^{(2)}_{\rm eff}$, a key point is how to re-describe Levy's density functional, $F[n]$, by a model functionals. The solution is given below.

$$F[n] = T_0[n] + V_{\rm ee}[n] + E_{\rm rxc}[n] \tag{3}$$

$$T_0[n] = \langle\Psi|\left[\sum_{ij\sigma}\int d^3r\phi_{i\sigma}(\mathbf{r})\left(-\frac{\hbar^2}{2m}\Delta\right)\phi_{j\sigma}(\mathbf{r})c^\dagger_{i\sigma}c_{j\sigma}\right]|\Psi\rangle \tag{4}$$

$$V_{\rm ee}[n] = \frac{1}{2}\int\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}n(\mathbf{r})n(\mathbf{r}')d^3rd^3r' + {\sum_{ijkl\sigma\sigma'}}'\frac{1}{2}\int\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\phi^*_{i\sigma}(\mathbf{r})\phi^*_{j\sigma'}(\mathbf{r}')\phi_{k\sigma'}(\mathbf{r}')\phi_{l\sigma}(\mathbf{r})d^3rd^3r'\bar{\rho}^{(2)}(ijkl;\sigma\sigma') \tag{5}$$

Here the two-particle density matrix, $\bar{\rho}^{(2)}(ijkl;\sigma\sigma')$, is defined using the single-particle density matrix, $\rho(ij;\sigma) = \langle\Psi|c^\dagger_{i\sigma}c_{j\sigma}|\Psi\rangle$, as follows.

$$\bar{\rho}^{(2)}(ijkl;\sigma\sigma') = \langle\Psi|c^\dagger_{i\sigma}c^\dagger_{j\sigma'}c_{k\sigma'}c_{l\sigma}|\Psi\rangle - \rho(il;\sigma)\rho(jk;\sigma')$$

A residual many-particle interaction, $\hat{H}_{\rm rxc}$, is a kind of the exchange-correlation correction coming from definitions of both $E_{\rm rxc}[n]$ and $v_{\rm eff}(\mathbf{r})$ and is defined as,

$$\langle\Psi|\hat{H}_{\rm rxc}|\Psi\rangle = E_{\rm rxc}[n] - \int\frac{\delta E_{\rm rxc}}{\delta n(\mathbf{r})}n(\mathbf{r})d^3r$$

In our new scheme, a summation, $\sum'$, appearing in two-particle interactions is arbitrary. Thus, our formulation is applicable for description of any type of local interactions including the Hubbard interaction. Although an additional approximation on the new exchange-correlation term, $E_{\rm rxc}$, is required, our scheme provides the Hubbard model, the Anderson-lattice model *etc.* starting from DFT without artificial inclusion of the U-term as performed in the LDA+U approach. If $\sum'$ is taken for all possible terms, $E_{\rm rxc}[n] \equiv 0$. This property may be useful to discuss the v-representability problem remaining in the original Kohn-Sham theory.

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